Generalized Linear Polyominoes, Green functions and Green matrices

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Abstract. In this work we derive the Green function of a generalized linear Polyomino as a suitable perturbation of the Green function of a Hamiltonian path on it. So, our study encompasses previous works on polyomino–like chains.

Key words: Linear Polyominoes, Green function, Green matrices.

1 Introduction

A Polyomino is an edge–conected union of cells in the planar square lattice. Quoting [8], "Polyominoes have a long history, going back to the start of the 20th century, but they were popularized in the present era initially by Solomon Golomb, then by Martin Gardner in his *Scientific American* columns "Mathematical Games". They now constitute one of the most popular subjects in mathematical recreations, and have found interest among mathematicians, physicists, biologists, and computer scientists as well." Because the chemical constitution of a molecule is conventionally represented by a molecular graph or network, the polyominoes have deserved the attention of the Organic Chemistry community. So, several molecular structure descriptors based in network structural descriptors, have been introduced, see for instance [13]. In particular, in the last decade a great amount of works devoted to calculate the Kirchhoff Index of linear polyominoes-like networks, have been published, see [12] and references therein. In this work we deal with this class of polyominoes, that we call generalized linear polyominoes, that besides the most popular class of linear polyomino chains, also includes cycles, Phenylenes and Hexagonal chains to name only a few. Because the Kirchhoff Index is the trace of the Green function of the network, see [1], here we obtain the Green function of

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such a networks. To do this, we understand a polyomino as a perturbation of a path by adding weighted edges between opposite vertices. Therefore, unlike the techniques used in [12], that are based on the decomposition of the combinatorial Laplacian in structured blocks, here we obtain the Green function of a linear polyomino from a perturbation of the combinatorial Laplacian. This approach deeply link linear polyomino Green functions with the inverse M-matrix problem an very specially with the so-called Green matrices.

The oldest class of symmetric, inverse M-matrices is the class of positive *type D* matrices defined by Markham [9]. A $s \times s$ matrix $\Sigma = (\sigma_{ij})$ is of type D if there exist real numbers $\{\sigma_i\}_{i=1}^n$, with $\sigma_n > \sigma_{n-1} > \ldots > \sigma_1$, such that $\sigma_{ij} = \sigma_{\min\{i,j\}}$. In the same work, it was proved that if $\sigma_1 > 0$ then Σ^{-1} is a tridiagonal M-matrix. The matrix Σ is named of *weak type D* if there are no constrain on the parameters $\{\sigma_i\}_{i=1}^n$.

On the other hand, a $s \times s$ *flipped weak type D* matrix with parameters $\{\sigma_i\}_{k=1}^s$ is the matrix $\Sigma = (\sigma_{ij})$ whose entries satisfy $\sigma_{ij} = \sigma_{\max\{i,j\}}$. When, in addition, the parameters satisfy $\sigma_1 > \cdots > \sigma_s$, then Σ is named a *flipped type D* matrix. In this work we will use the following result on flipped weak type D matrices, whose proof is straightforward, see also [10].

Lemma 1. *Consider Σ the $s \times s$ flipped weak type D matrix with parameters $\sigma_1, \ldots, \sigma_s$ and define $\sigma_{s+1} = 0$. Then Σ is invertible iff the parameters satisfy $\sigma_j \neq \sigma_{j+1}$, $j = 1, \ldots, s$ and when this condition holds, then Σ^{-1} is the tridiagonal matrix*

$$\Sigma^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 & 0 \\ -\gamma_1 & \gamma_1 + \gamma_2 & -\gamma_2 & \cdots & 0 & 0 \\ 0 & -\gamma_2 & \gamma_2 + \gamma_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_{s-2} + \gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1} + \gamma_s \end{bmatrix},$$

where $\gamma_j = \dfrac{1}{\sigma_j - \sigma_{j+1}}$, $j = 1, \ldots, s$. Moreover, Σ^{-1} is a Z-matrix iff Σ is an $s \times s$ flipped type D matrix and an M-matrix when, in addition $\sigma_s > 0$.

A *Green* matrix, G is defined as the Hadamard product $\mathsf{G} = \mathsf{A} \circ \mathsf{B}$, of a weak type D matrix, A, and a flipped weak type D matrix, B, see [10]. A classical result by Gantmacher and Krein, see [7], states that G is a nonsingular Green matrix iff G^{-1} is an irreducible tridiagonal matrix.

2 Generalized Linear Polyominoes

We consider a fixed path P on $2n$ vertices, labeled as $V = \{x_1, \ldots, x_{2n}\}$. The class of (generalized) *Linear Polyomino* supported by the path P, denoted by

$\mathbb{L}_n$, see [12], consists of all connected networks whose conductance satisfies that $c_i = c(x_i, x_{i+1}) > 0$ for $i = 1, \dots, 2n-1$, $a_i = c(x_i, x_{2n+1-i}) \geq 0$ for any $i = 1, \dots, n-1$ and $c(x_i, x_j) = 0$ otherwise. Clearly if $\mathcal{P} \in \mathbb{L}_n$, P is a Hamiltonian path in $\mathcal{P}$.

We define the *link number* of $\mathcal{P} \in \mathbb{L}_n$ as $s = |\{i = 1, \dots, n-1 : a_i > 0\}|$. So, the link number of $\mathcal{P} \in \mathbb{L}_n$ equals 0 iff $a_1 = \dots = a_{n-1} = 0$, that is, iff the underlying graph of $\mathcal{P}$ is nothing but the path P. On the other hand, if the link number of $\mathcal{P}$ is positive there exist a sequence $1 \leq i_1 < \dots < i_s \leq n-1$, called *link sequence of* $\mathcal{P}$, such that $a_{i_k} > 0$ when $k = 1, \dots, s$, whereas $a_k = 0$ otherwise, see Figure 1.

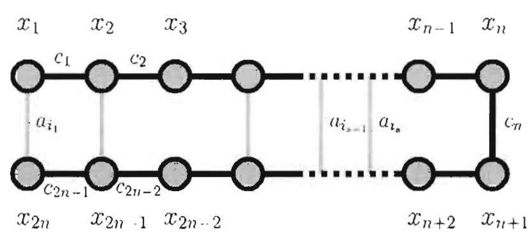

Fig. 1. Linear Polyomino Chain

Among the polyominoes supported by P are the cycles with vertex set V, which correspond to the case $a_1 > 0$ and $a_j = 0$, $j = 2, \dots, n-1$. In addition, we next describe some examples of linear polyominoes with positive link number that have been considered in the framework of Organic Chemistry. A polyomino whose link number equals $n-1$ is called a *linear polyomino chain* and the class of these polyominoes is usually represented as $\mathcal{L}_{n-1}$. In particular, when $c_j = c_{2n-j}$, and $a_j = c_n$, $j = 1, \dots, n-1$, the linear polyomino chain appears as the Cartesian product of the path on $\{x_1, \dots, x_n\}$ with conductances c_j, $j = 1, \dots, n-1$ and the complete network on two vertices with conductance c_n.

When $n = 3m$, $a_{3k-1} = 0$ for any $k = 1, \dots, m$ and $a_j > 0$, otherwise, then $\mathcal{P}$ is called *linear Phenylene*, its link number equals $2m-1$ and it is represented as PH_m, see Figure 2.

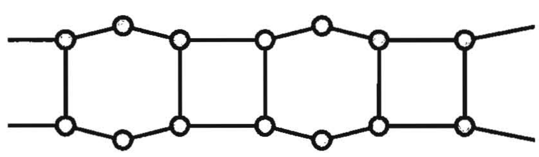

Fig. 2. Phenylene.

When $n = 2m+1$, $a_{2k} = 0$ for any $k = 1, \dots, m$ and $a_j > 0$, otherwise, then the general polyomino is called linear Hexagonal chain, see Figure 3 and it is represented as L_m.

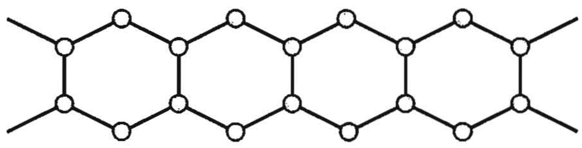

Fig. 3. HexagonalChain.

Given $\mathcal{P} \in \mathbb{L}_n$, we denote its Green function as $G^{\mathcal{P}}$. If $\mathcal{P}$ as positive link number s and $\{i_j\}_{j=1}^{s}$ is its link sequence, then the combinatorial Laplacian of $\mathcal{P}$ appears as the combinatorial Laplacian of the weighted Hamiltonian path perturbed by adding for all $j = 1, \dots, s$ an edge with conductance a_{ij} between vertices x_{i_j} and x_{2n+1-i_j}.

Consider $\mathcal{G}$ and G, the Green operator and the Green function of the path P, and for $j = 1, \dots, s$ the dipole $\sigma_j = \sqrt{a_{i_j}}(\varepsilon_{x_{i_j}} - \varepsilon_{x_{2n+1-i_j}})$, where ε_x denotes the Dirac function at vertex x and the function $\mathcal{G}(\sigma_j)$. We get the following result, see [2].

Theorem 1. *Let the $(s \times s)$-matrices $\mathsf{\Lambda} = \big(\langle \mathcal{G}(\sigma_j), \sigma_k \rangle\big)$ and $\mathsf{I} + \mathsf{\Lambda}$. Then, $\mathsf{I} + \mathsf{\Lambda}$ is non singular and*

$$G^{\mathcal{P}}(x_i, x_j) = G(x_i, x_j) - \sum_{k,m=1}^{s} b_{km} \mathcal{G}(\sigma_k)(x_i) \mathcal{G}(\sigma_k)(x_j), \quad i, j = 1, \dots, 2n.$$

where $(b_{km}) = (\mathsf{I} + \mathsf{\Lambda})^{-1}$.

The rest of this work is devoted to obtain the matrix $\mathsf{\Lambda}$ and to calculate $(b_{km}) = (\mathsf{I} + \mathsf{\Lambda})^{-1}$.

The expression of the Green function G of the Hamiltonian path, was obtained in [4] and is

$$G(x_i, x_j) = \frac{1}{2n} \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{k^2}{c_k} + \sum_{k=\max\{i,j\}}^{2n-1} \frac{(2n-k)^2}{c_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{k(2n-k)}{c_k} \right]$$

where we use the convention $\sum\limits_{l=i}^{j} \alpha_l = 0$ when $j < i$. In addition, the effective resistance between x_i and x_j is

$$R(x_i, x_j) = 2n \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{c_k}.$$

Observe that for $i \le j$ we get

$$R(x_i, x_{2n+1-i}) = R(x_i, x_j) + R(x_j, x_{2n+1-j}) + R(x_{2n+1-j}, x_{2n+1-i})$$

In addition, for $j = 1, \dots, s$

$$\mathcal{G}(\sigma_j)(x_m) = \sqrt{a_{ij}}\left[2n \sum_{k=\max\{m,i_j\}}^{2n-i_j} \frac{1}{c_k} - \sum_{k=i_j}^{2n-i_j} \frac{k}{c_k}\right], \quad m = 1, \dots, 2n,$$

and hence, for $k = 1, \dots, s$,

$$\langle \mathcal{G}(\sigma_j), \sigma_k \rangle = \sqrt{a_{i_j} a_{i_k}} R(x_{\max\{i_j,i_k\}}, x_{2n+1-\max\{i_j,i_k\}}).$$

If D is the diagonal matrix whose diagonal entries are $a_{i_1}, \dots, a_{i_s}$, then $\mathsf{D}^{-\frac{1}{2}}(\mathsf{I} + \Lambda)\mathsf{D}^{-\frac{1}{2}} = \mathsf{D}^{-1} + \mathsf{A}$, where

$$\mathsf{A} = \begin{bmatrix} R(x_{i_1}, x_{2n+1-i_1}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ R(x_{i_2}, x_{2n+1-i_2}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ \vdots & \vdots & \ddots & \vdots \\ R(x_{i_s}, x_{2n+1-i_s}) & R(x_{i_s}, x_{2n+1-i_s}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \end{bmatrix}.$$

So, A is a $s \times s$ flipped type D matrix with parameters $\{R(x_{i_k}, x_{2n+1-i_k})\}_{k=1}^{s}$, because $R(x_1, x_{2n+1-1}) > \cdots > R(x_{n-1}, x_{n+1}) > 0$. Therefore, applying Lemma 1, A^{-1} is the tridiagonal M-matrix

$$\mathsf{A}^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 & 0 \\ -\gamma_1 & \gamma_1 + \gamma_2 & -\gamma_2 & \cdots & 0 & 0 \\ 0 & -\gamma_2 & \gamma_2 + \gamma_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_{s-2} + \gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1} + \gamma_s \end{bmatrix},$$

where $\gamma_s = \dfrac{1}{R(x_{i_s}, x_{2n+1-i_s})}$ and $\gamma_k = \dfrac{1}{R(x_{i_k}, x_{i_{k+1}}) + R(x_{2n+1-i_{k+1}}, x_{2n+1-i_k})}$, $k = 1, \dots, s-1$. Clearly, $\mathsf{A}^{-1} + \mathsf{D}$ is a strictly diagonally dominant tridiagonal M-matrix and hence it is invertible and moreover $(\mathsf{A}^{-1} + \mathsf{D})^{-1} > 0$. In addition, $\mathsf{I} + \Lambda = \mathsf{D}^{\frac{1}{2}}(\mathsf{D}^{-1} + \mathsf{A})\mathsf{D}^{\frac{1}{2}} = \mathsf{D}^{\frac{1}{2}}\mathsf{A}(\mathsf{A}^{-1} + \mathsf{D})\mathsf{D}^{-\frac{1}{2}}$ and hence,

$$\begin{aligned}(\mathsf{I} + \Lambda)^{-1} &= \mathsf{D}^{\frac{1}{2}}\left[\mathsf{A}^{-1} + \mathsf{D}\right]^{-1}\mathsf{A}^{-1}\mathsf{D}^{-\frac{1}{2}} \\ &= \mathsf{D}^{\frac{1}{2}}\left[\mathsf{I} - (\mathsf{A}^{-1} + \mathsf{D})^{-1}\mathsf{D}\right]\mathsf{D}^{-\frac{1}{2}} = \mathsf{I} - \mathsf{D}^{\frac{1}{2}}(\mathsf{A}^{-1} + \mathsf{D})^{-1}\mathsf{D}^{\frac{1}{2}}\end{aligned}$$

and we only need to calculate $(\mathsf{A}^{-1} + \mathsf{D})^{-1}$.

When $s=1$, then $\gamma_1 = \dfrac{1}{R(x_{i_1}, x_{2n+1-i_1})}$, $(\mathsf{A}^{-1}+\mathsf{D})^{-1} = \dfrac{1}{\gamma_1 + a_{i_1}}$ and hence $(\mathsf{I}+\Lambda)^{-1} = \dfrac{\gamma_1}{\gamma_1 + a_{i_1}} = \dfrac{1}{1 + a_{i_1} R(x_{i_1}, x_{2n+1-i_1})}$.

When $s \geq 2$, $\mathsf{A}^{-1}+\mathsf{D}$ is a tridiagonal matrix so we can apply the results involving this class of matrices, see for instance [11]. In addition, we can also apply the usual techniques for discrete boundary value problems, see [5,6]. Specifically, we have the following result expressing the entries of $\mathsf{A}^{-1}+\mathsf{D}$ and hence the entries of $(\mathsf{I}+\Lambda)^{-1}$ in terms of the solutions of two difference equations. In particular, we obtain that $\mathsf{A}^{-1}+\mathsf{D}$ is a Green matrix as Gantmacher & Krein's theorem assures.

Proposition 1. *When the link number s satisfies that $s \geq 2$, consider $\{u_j\}_{j=1}^s$ and $\{v_j\}_{j=1}^s$ the solutions of the different equation*

$$\big(a_{i_k} + \gamma_{k-1} + \gamma_k\big) z_k - z_{k-1}\gamma_{k-1} - z_{k+1}\gamma_k = 0, \quad k = 2, \ldots, s-1,$$

characterized by satisfying the initial conditions $u_1 = \gamma_1$, $u_2 = a_{i_1} + \gamma_1$ and the final conditions $v_{s-1} = a_{i_s} + \gamma_s + \gamma_{s-1}$, $v_s = \gamma_{s-1}$, respectively. Then, $\gamma_1 v_2 \neq (a_{i_1} + \gamma_1) v_1$ and moreover

$$b_{jk} = \delta_{jk} - \frac{\sqrt{a_{i_j} a_{i_k}}}{\gamma_1\big((a_{i_1} + \gamma_1)v_1 - \gamma_1 v_2\big)} u_{\min\{j,k\}} v_{\max\{j,k\}}, \qquad j,k = 1, \ldots, s.$$

When $s \leq 3$ we can solve explicitly the above equations. For $s \geq 4$, several hypotheses can be made on the coefficients of the difference equation in proposition 1 in order to calculate explicitly the sequences $\{u_j\}_{j=1}^s$ and $\{v_j\}_{j=1}^s$. In the next section we assume the simplest one, namely that all coefficients are constant.

3 Self–complementary Polyominoes

A polyomino $\mathcal{P} \in \mathbb{L}_n$ with link number $s \geq 3$ and link sequence $\{i_j\}_{j=1}^s$ is called *self-complementary* if there exist $a, r_1, r_2 > 0$ such that

$$a_{i_j} = a, \quad r_1 = R(x_{i_j}, x_{i_{j+1}}) \quad \text{and} \quad r_2 = R(x_{2n+1-i_{j+1}}, x_{2n+1-i_j})$$

for all $j = 1, \ldots, s-1$, where is the link sequence of $\mathcal{P}$. Moreover, the value $q = 1 + \dfrac{ar}{2}$, where $r = r_1 + r_2$, is called the *potential of $\mathcal{P}$*.

A linear Polyomino chain is self–complementary iff $a_j = a$, $c_j = r_1^{-1}$ and $c_{2n-j} = r_2^{-1}$, $1 \leq j \leq n-1$.

A Phenylene is self–complementary iff $a_{3j-2} = a_{3j} = a$, $c_{3j} = \dfrac{1}{r_1}$, $c_{3(2m-j)} = \dfrac{1}{r_2}$, $j = 1, \ldots, m-1$, $\dfrac{1}{c_{3j-2}} + \dfrac{1}{c_{3j-1}} = r_1$ and $\dfrac{1}{c_{3(2m-j)+2}} + \dfrac{1}{c_{3(2m-j)+1}} = r_2$, $j = 1, \ldots, m$.

An Hexagonal Chain is self–complementary iff $a_{2j-1} = a_{2j+1} = a$ for all $j = 1, \dots, m-1$, $\dfrac{1}{c_{2j-1}} + \dfrac{1}{c_{2j}} = r_1$ and $\dfrac{1}{c_{2(2m+1-j)+1}} + \dfrac{1}{c_{2(2m+1-j)}} = r_2$, $j = 1, \dots, m$.

If we consider fixed the link number $s \geq 3$ and the link sequence $\{i_j\}_{j=1}^{s}$, then the corresponding set of self–complementary polyominoes depends on $2(n+2-s)$ parameters. Moreover, the difference equation in Proposition (1) becomes

$$z_{i+1} = 2qz_i - z_{i-1}, \quad i = 2, \dots, n-2$$

and hence its solutions are of the form $z_i = \alpha U_{i-1}(q) + \beta U_i(q)$, where U_i is the i–th Chebyshev polynomial of second kind, see [5]. Therefore, if V_i denotes the i–th Chebyshev polynomial of third kind; that is $V_i = U_i - U_{i-1}$, with the notations of Proposition 1, for $i = 1, \dots, s$ we get

$$u_i = \frac{1}{r} V_{i-1}(q) \quad \text{and} \quad v_i = \frac{\Big[R(x_s, x_{2n+1-s})V_{s-i}(q) + rU_{s-1-i}(q)\Big]}{rR(x_s, x_{2n+1-s})},$$

and hence for $i, j = 1, \dots, s$,

$$b_{jk} = \delta_{jk} - \frac{aV_{\min\{j,k\}-1}(q)\big[R(x_s, x_{2n+1-s})V_{s-\max\{j,k\}}(q) + rU_{s-1-\max\{j,k\}}(q)\big]}{R(x_s, x_{2n+1-s})\big[aU_{s-1}(q) + V_{s-1}(q)\big]}.$$

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